Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1611txm

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

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* * * * * * * * * *
                     Welcome to STN International
NEWS
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
                 "Ask CAS" for self-help around the clock
                 CA/CAplus records now contain indexing from 1907 to the
NEWS
         SEP 09
                 present
         AUG 05 New pricing for EUROPATFULL and PCTFULL effective
NEWS
                 August 1, 2003
        AUG 13
                Field Availability (/FA) field enhanced in BEILSTEIN
NEWS 5
NEWS 6 AUG 18
                 Data available for download as a PDF in RDISCLOSURE
NEWS 7 AUG 18
                 Simultaneous left and right truncation added to PASCAL
NEWS 8 AUG 18 FROSTI and KOSMET enhanced with Simultaneous Left and Righ
                 Truncation
NEWS 9 AUG 18
                 Simultaneous left and right truncation added to ANABSTR
NEWS 10
        SEP 22
                 DIPPR file reloaded
NEWS 11
        SEP 25
                 INPADOC: Legal Status data to be reloaded
NEWS 12
        SEP 29
                 DISSABS now available on STN
NEWS 13
         OCT 10
                 PCTFULL: Two new display fields added
NEWS 14 OCT 21
                 BIOSIS file reloaded and enhanced
NEWS 15 OCT 28 BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS EXPRESS NOVEMBER 14 CURRENT WINDOWS VERSION IS V6.01c, CURRENT
              MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
              AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003
NEWS HOURS
              STN Operating Hours Plus Help Desk Availability
              General Internet Information
NEWS INTER
NEWS LOGIN
              Welcome Banner and News Items
              Direct Dial and Telecommunication Network Access to STN
NEWS PHONE
NEWS WWW
              CAS World Wide Web Site (general information)
```

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 10:57:45 ON 24 NOV 2003

=> file casreacts

'CASREACTS' IS NOT A VALID FILE NAME SESSION CONTINUES IN FILE 'HOME'

Enter "HELP FILE NAMES" at an arrow prompt (=>) for a list of files that are available. If you have requested multiple files, you can specify a corrected file name or you can enter "IGNORE" to continue accessing the remaining file names entered.

=> file casreact COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

FILE 'CASREACT' ENTERED AT 10:58:18 ON 24 NOV 2003 USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE CONTENT: 1907 - 23 Nov 2003 VOL 139 ISS 21

Some records from 1974 to 1991 are derived from the ZIC/VINITI data file and provided by InfoChem and some records are produced using some INPI data from the period prior to 1986.

This file contains CAS Registry Numbers for easy and accurate substance identification.

Crossover limits have been increased. See HELP RNCROSSOVER for details.

Structure search limits have been raised. See HELP SLIMIT for the new, higher limits.

=>

Uploading C:\Program Files\Stnexp\Queries\10087112.str

chain nodes :

12 13 14 15 21 22 34 35 36 37 39 40 42 43 16 17 18 19 20 38 41 44 45 46 47 48 51

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 23 24 25 26 27 28 29 30 31 32 33 chain bonds : 1-8 2-13 4-12 6-20 8-19 9-18 9-46 10-17 10-45 11-14 11-16 14-15 14-21 14-22 15-51 23-30 24-35 26-34 28-42 30-41 31-40 32-39 33-36 33-38 36-37 36-43 36-44 45-47 46-48 ring bonds : 1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-11 8-9 9-10 10-11 23-24 23-28 24-25 25-26 26-27 27-28 29-30 29-33 30-31 31-32 32-33 exact/norm bonds : 1-2 1-6 1-8 2-3 2-13 3-4 4-5 4-12 5-6 7-8 7-11 8-9 9-10 9-46 10-11 10-45 14-15 23-24 23-28 23-30 24-25 24-35 25-26 26-27 26-34 27-28 29-30 29-33 30-31 31-32 32-33 36-37 exact bonds : 6-20 8-19 9-18 10-17 11-14 11-16 14-21 14-22 15-51 28-42 30-41 31-40 32-39 33-36 33-38 36-43 36-44 45-47 46-48

## Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 51:CLASS fragments assigned product role: containing 23 fragments assigned reactant/reagent role: containing 1

## L1 STRUCTURE UPLOADED

=> s l1 sample SAMPLE SEARCH INITIATED 10:58:42 FILE 'CASREACT' SCREENING COMPLETE - 434 REACTIONS TO VERIFY FROM 37 DOCUMENTS

0 DOCS 100.0% DONE 434 VERIFIED 0 HIT RXNS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\* BATCH \*\*COMPLETE\*\* PROJECTED VERIFICATIONS: 7431 TO 9929 PROJECTED ANSWERS: O TO

L2 0 SEA SSS SAM L1 ( 0 REACTIONS)

=> s 11 full FULL SEARCH INITIATED 10:58:51 FILE 'CASREACT' SCREENING COMPLETE - 6907 REACTIONS TO VERIFY FROM 517 DOCUMENTS

100.0% DONE 6907 VERIFIED 3 HIT RXNS 2 DOCS SEARCH TIME: 00.00.01

2 SEA SSS FUL L1 ( 3 REACTIONS) L3

=> d 1-2

Page 3

## ANSWER 1 OF 2 CASREACT COPYRIGHT 2003 ACS on STN L3

RX(6) OF 9 - 2 STEPS

1.1. Me2C(OAc)COBr, AcOEt, MeCN

1.2. KHCO3, Water
2.1. CuSO4, Zn, Water
2.2. AcOH, DMF

2.3. K2CO3, Water

RX(6) OF 9 - 2 STEPS

85%

REF: PCT Int. Appl., 2002070533, 12 Sep 2002 NOTE: 1) optimization study, combined yield of 88%, 2) optimized on solvent, first stage prepn. of reducing agent

ANSWER 2 OF 2 CASREACT COPYRIGHT 2003 ACS on STN L3

RX(47) OF 58 - 5 STEPS

- 1.1. Pivaloyl chloride, Pyridine
- 1.2. MeSO2Cl
- Mg (OMe) 2, NaBH4,
   N2, Benzene, MeOH
- 3. Pivaloyl chloride, Pyridine
- 4. TsCl, NaH, THF
- 5.1. t-BuOK, t-BuOH
- 5.2. NH3, MeOH

REF: Chemistry Letters, (12), 2419-22; 1987

=> logoff

ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y)/N/HOLD:.

COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 103.15 103.36

FULL ESTIMATED COST

STN INTERNATIONAL LOGOFF AT 10:59:30 ON 24 NOV 2003

| L Number | Hits | Search Text                               | DB       | Time stamp       |
|----------|------|---|----------|------------------|
| 1        | 554  | (544/317).CCLS.                           | USPAT;   | 2003/11/24 08:58 |
| 1        |      |   | US-PGPUB |                  |
| 2        | 8    | ((544/317).CCLS.) and (couple or "Zn/Cu") | USPAT;   | 2003/11/24 11:43 |
|          |      |   | US-PGPUB |                  |
| 3        | 27   | ((544/317).CCLS.) and ("5-fluoro")        | USPAT;   | 2003/11/24 11:43 |
| 1        |      |   | US-PGPUB |                  |